

Lawrence Livermore Laboratory

PRODUCTION OF MULTI-GROUP DATA AT LIVERMORE

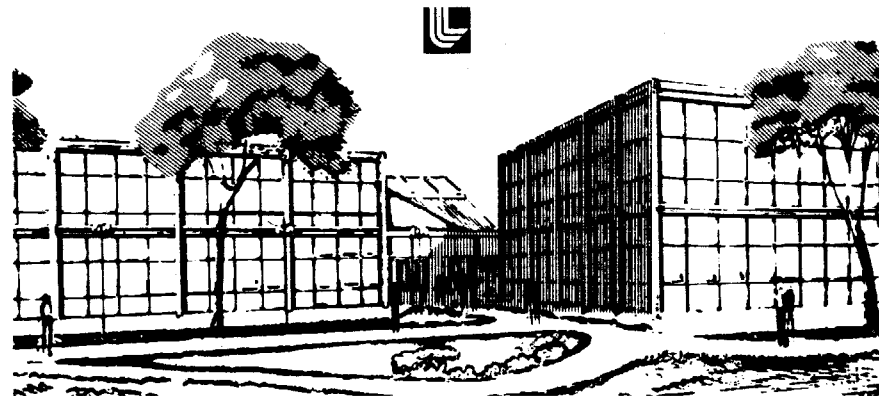
Peter C. Giles

March 1978

CIRCULATION COPY
SUBJECT TO RECALL
IN TWO WEEKS

This paper was prepared for submission to the Radiation Shielding Information Center (RSIC) Seminar-Workshop, held at Oak Ridge, Tennessee, March 14-16, 1978.

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint is made available with the understanding that it will not be cited or reproduced without the permission of the author.



DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

Best Available Quality

for original report

**call
Reports Library**

X37097

PRODUCTION OF MULTI-GROUP DATA AT LIVERMORE*

Peter C. Giles
Lawrence Livermore Laboratory
Livermore, California, U.S.A.

ABSTRACT

The Livermore evaluated nuclear data library (ENDL) is used at Livermore as a source of data from which multi-group parameters are derived for use in a variety of transport codes which in terms of methods span the gamut from Monte Carlo to S_n to diffusion and in terms of particles considered includes neutrons, photons and/or charged particles.

In order to service all of these application areas a system of computer codes have been in operation for some time. This paper will discuss the initial design philosophy and goals of this system, its present status and future projected features.

The CLYDE code has been developed to handle a broad range of cross section processing requirements. These run the gamut of data tables for Monte Carlo to S_n to Diffusion codes. The present version processes neutron and gamma interactions from neutron-induced reactions. The code is operable on the CDC-7600, and occupies about 155k (octal) of SCM; 460k (octal) words of LCM are available for storage and working arrays.

The evaluated cross sections that are input to CLYDE may appear on either cards, tape, or disk, but they must be in the format of the Evaluated Nuclear Data Library (ENDL). ENDL is described in LLL report UCRL-50400, Vol. 4 (1971). Furthermore, the user must specify group boundaries, weighting fluxes, and the isotopes for which the processed data are required. The atomic mass for each isotope is carried with the isotope in the evaluated library. Standard sets of group boundaries and weighting fluxes are also maintained. There is, incidentally, a preprocessor (ENDFLLL) available to translate ENDF/B library data into the ENDL input format, and vice versa.

The output from CLYDE is flux-averaged group cross sections, transfer probabilities, energy depositions, particle and isotope cross sections, isotope destruction cross sections, and appropriate averages of collateral quantities such as the average number of neutrons per fission. The code

*Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore Laboratory under contract number W-7405-ENG-48.

processes data for transport theory, diffusion theory or Monte Carlo applications to neutronic systems, shielding, and fusion research.

The design philosophy behind the CLYDE code encompasses these points:

- a) It is designed to be unlimited in the amount of data it can handle, and in the number of groups and order of transfer matrices that it can generate.
- b) It is designed to calculate the group constants for any isotope with a standard group structure and scattering order in a reasonable amount of computer time.
- c) Built-in rigidity with regard to particular models or parameters is not allowed.
- d) Redundancy in input information is allowed in the evaluated library, but is not processed in CLYDE.
- e) Output is provided in two general formats for the S_n/D_n (deterministic) codes. CTART produces Monte Carlo output. Card, disc, or tape output are all available, and with each option printouts are produced that include all pertinent information in a convenient form.

Conditions (b) and (c) are satisfied by transferring certain specific model calculations to preprocessor codes. These codes perform appropriate operations to produce basic microscopic data from models and/or recipes. Their results are stored in ENDL. Or these results may be used as card input to CLYDE if it is undesirable to place them in the library. Some of these preprocessor functions are:

- a) To convert angular distributions to Legendre coefficients, incorporating fitting and thinning procedures (UPDATE).
- b) To process scattering kernels for the more time-consuming multibody transfer processes (e.g., $n, 2n$); and, to generate the correlated energy-angle Legendre expansions of the kernels (FIRST and DECAY).
- c) To generate thermal scattering kernels from $S(\alpha, \beta)$ data (FLANGELL).
- d) To generate differential angular probability data from Legendre expansion coefficients (UPDATE).
- e) To generate energy tables for the emitted neutrons from fission (FISPEC).
- f) To calculate average energy depositions from neutron induced reactions (ENDEP).

- g) To generate "cold" cross section data from resonance parameters (resolved or unresolved) (ENDFLL).

Where is CLYDE going? We will be elaborating our charged particle interaction file (presently an addendum to ENDL). Part of the user community at LLL is interested in charged particle scattering matrices for both scattered particle and knockon, and for other appropriate group constants (e.g., reaction cross sections). EGDL is the gamma analogue to the ENDL file. We intend that CLYDE be able to operate on EGDL and ENDL files to produce a complete set of nuclear group constants, whether neutron, gamma, or charged particle initiated. It now handles neutron and photon data. For charged particles, our initial efforts include data for the hydrogen and helium isotopes. We may proceed in Z beyond that, thinking, for example, of potential medical physics requirements.

Plans for CLYDE also include an abbreviated operation which would provide activation group constants; essentially the usual reaction and destruction cross sections, but without transfer matrices. The base data file (ACTL) presently exists.

Other improvements include an improved Doppler broadening subroutine (SIGMAL). We may try to include some kind of Bonderenko self-shielding.

Finally, there are some almost "cosmetic" improvements which need to be made. We expect to realize some timing improvement, especially with higher order output. We now use double, even triple precision routines for some of our integrals. We have available some more sophisticated algorithms which require only single precision, and which should be implemented soon. Lastly, CLYDE is a user code. Unless program proprietors want to become involved in every users dalliance with their code, it is essential that simple instructions, complete diagnostic and error comments, and reasonable drop-through options be provided. We intend to put considerable effort into these last items.

NOTICE

"This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights."

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.